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Table S1. Bond Distances (Å) and Angles (deg) for (η^4-C_5Bz_5H)Fe(CO)$_3$.

Atoms	Distance	Atoms	Distance
Fe -- C(1)	1.807(7)	Fe -- C(2)	1.792(6)
Fe -- C(3)	1.777(6)	Fe -- C(4)	2.130(5)
Fe -- C(5)	2.067(5)	Fe -- C(6)	2.062(6)
Fe -- C(7)	2.105(5)	O(1) -- C(1)	1.142(9)
O(2) -- C(2)	1.126(7)	O(3) -- C(3)	1.143(8)
C(4) -- C(5)	1.437(9)	C(4) -- C(8)	1.515(6)
C(4) -- C(9)	1.508(8)	C(5) -- C(6)	1.427(7)
C(5) -- C(16)	1.504(7)	C(6) -- C(7)	1.441(8)
C(6) -- C(23)	1.53(1)	C(7) -- C(8)	1.514(8)
C(7) -- C(30)	1.497(7)	C(8) -- C(37)	1.569(7)
C(9) -- C(10)	1.51(1)	C(10) -- C(11)	1.388(8)
C(10) -- C(15)	1.383(9)	C(11) -- C(12)	1.38(1)
C(12) -- C(13)	1.37(1)	C(13) -- C(14)	1.38(1)
C(14) -- C(15)	1.38(1)	C(16) -- C(17)	1.514(8)
C(17) -- C(18)	1.363(9)	C(17) -- C(22)	1.38(1)
C(18) -- C(19)	1.387(9)	C(19) -- C(20)	1.38(1)
C(20) -- C(21)	1.35(1)	C(21) -- C(22)	1.377(9)
C(23) -- C(24)	1.529(8)	C(24) -- C(25)	1.368(8)
C(24) -- C(29)	1.367(9)	C(25) -- C(26)	1.38(1)
C(26) -- C(27)	1.35(1)	C(27) -- C(28)	1.37(1)
C(28) -- C(29)	1.36(1)	C(30) -- C(31)	1.516(9)
C(31) -- C(32)	1.376(9)	C(31) -- C(36)	1.397(9)
C(32) -- C(33)	1.38(1)	C(33) -- C(34)	1.38(1)
C(34) -- C(35)	1.39(1)	C(35) -- C(36)	1.38(1)
C(37) -- C(38)	1.523(9)	C(38) -- C(39)	1.387(8)

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Table S1. continued

C(38) -- C(43)	1.37(1)	C(39) -- C(40)	1.40(1)
C(40) -- C(41)	1.34(1)	C(41) -- C(42)	1.36(1)
C(42) -- C(43)	1.38(1)	Cent[a] -- Fe	1.72

Atoms	Angle	Atoms	Angle
C(1) -- Fe -- C(2)	100.3(3)	C(1) -- Fe -- C(3)	100.1(3)
C(2) -- Fe -- C(3)	91.8(3)	Fe -- C(1) -- O(1)	177.9(5)
Fe -- C(2) -- O(2)	177.9(5)	Fe -- C(3) -- O(3)	177.9(5)
C(5) -- C(4) -- C(8)	108.4(5)	C(5) -- C(4) -- C(9)	122.7(4)
C(8) -- C(4) -- C(9)	123.7(5)	C(4) -- C(5) -- C(6)	106.0(4)
C(4) -- C(5) -- C(16)	127.2(5)	C(6) -- C(5) -- C(16)	126.7(6)
C(5) -- C(6) -- C(7)	107.5(5)	C(5) -- C(6) -- C(23)	127.3(5)
C(7) -- C(6) -- C(23)	125.1(5)	C(6) -- C(7) -- C(8)	107.0(4)
C(6) -- C(7) -- C(30)	123.5(6)	C(8) -- C(7) -- C(30)	123.2(4)
C(4) -- C(8) -- C(7)	96.4(4)	C(4) -- C(8) -- C(37)	115.4(4)
C(7) -- C(8) -- C(37)	111.1(5)	C(4) -- C(9) -- C(10)	117.0(4)
C(9) -- C(10) -- C(11)	119.5(5)	C(9) -- C(10) -- C(15)	121.8(5)
C(11) -- C(10) -- C(15)	118.6(6)	C(10) -- C(11) -- C(12)	121.0(6)
C(11) -- C(12) -- C(13)	119.4(6)	C(12) -- C(13) -- C(14)	120.5(8)
C(13) -- C(14) -- C(15)	119.8(7)	C(10) -- C(15) -- C(14)	120.6(6)
C(5) -- C(16) -- C(17)	114.1(4)	C(16) -- C(17) -- C(18)	121.7(6)
C(16) -- C(17) -- C(22)	121.0(5)	C(18) -- C(17) -- C(22)	117.3(5)
C(17) -- C(18) -- C(19)	122.5(7)	C(18) -- C(19) -- C(20)	118.2(7)
C(19) -- C(20) -- C(21)	120.6(6)	C(20) -- C(21) -- C(22)	119.9(7)
C(17) -- C(22) -- C(21)	121.5(6)	C(6) -- C(23) -- C(24)	111.4(5)
C(23) -- C(24) -- C(25)	120.6(5)	C(23) -- C(24) -- C(29)	122.1(5)
C(25) -- C(24) -- C(29)	117.3(6)	C(24) -- C(25) -- C(26)	121.3(6)

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Table S1. continued

C(25) -- C(26) -- C(27)	120.3(6)	C(26) -- C(27) -- C(28)	118.6(7)
C(27) -- C(28) -- C(29)	120.9(7)	C(24) -- C(29) -- C(28)	121.5(6)
C(7) -- C(30) -- C(31)	113.9(5)	C(30) -- C(31) -- C(32)	121.5(6)
C(30) -- C(31) -- C(36)	120.0(6)	C(32) -- C(31) -- C(36)	118.5(7)
C(31) -- C(32) -- C(33)	122.1(7)	C(32) -- C(33) -- C(34)	119.2(7)
C(33) -- C(34) -- C(35)	119.7(9)	C(34) -- C(35) -- C(36)	120.9(7)
C(31) -- C(36) -- C(35)	119.7(7)	C(8) -- C(37) -- C(38)	114.9(5)
C(37) -- C(38) -- C(39)	122.0(6)	C(37) -- C(38) -- C(43)	120.4(5)
C(39) -- C(38) -- C(43)	117.5(6)	C(38) -- C(39) -- C(40)	121.0(7)
C(39) -- C(40) -- C(41)	118.5(7)	C(40) -- C(41) -- C(42)	122.3(9)
C(41) -- C(42) -- C(43)	118.6(8)	C(38) -- C(43) -- C(42)	122.0(6)
Cent -- Fe -- C(1)	116.8	Cent -- Fe -- C(2)	120.9
Cent -- Fe -- C(3)	121.8		

[a]Cent is the centroid of the C4-C7 atomic positions.

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Table S2. Final Fractional Coordinates for (η^4-C_5Bz_5H)Fe(CO)$_3$.

Atom	x/a	y/b	z/c	B(eqv)a
Fe	0.86867(8)	0.60889(7)	0.84640(5)	2.05
O(1)	0.8300(5)	0.4496(4)	0.7291(3)	4.04
O(2)	0.6667(5)	0.5328(4)	1.0028(3)	4.41
O(3)	1.0877(5)	0.4396(5)	0.9053(3)	4.72
C(1)	0.8437(6)	0.5133(5)	0.7738(4)	2.73
C(2)	0.7461(6)	0.5600(5)	0.9427(4)	2.91
C(3)	1.0006(6)	0.5060(5)	0.8838(4)	2.93
C(4)	0.7614(5)	0.7767(5)	0.7905(3)	1.99
C(5)	0.8084(5)	0.8008(5)	0.8597(3)	2.02
C(6)	0.9512(5)	0.7732(5)	0.8334(3)	2.28
C(7)	0.9873(5)	0.7293(5)	0.7506(3)	1.97
C(8)	0.8739(5)	0.7856(5)	0.7086(3)	2.06
C(9)	0.6148(5)	0.7984(5)	0.7919(4)	2.52
C(10)	0.5669(5)	0.7019(5)	0.7556(4)	2.39
C(11)	0.5053(6)	0.6036(5)	0.8111(4)	2.70
C(12)	0.4572(7)	0.5154(6)	0.7801(5)	3.66
C(13)	0.4709(7)	0.5253(7)	0.6934(5)	4.26
C(14)	0.5288(7)	0.6241(7)	0.6374(4)	4.06
C(15)	0.5773(6)	0.7116(6)	0.6685(4)	2.97
C(16)	0.7247(6)	0.8486(5)	0.9421(3)	2.57
C(17)	0.6951(6)	0.9934(5)	0.9362(4)	2.52
C(18)	0.6561(7)	1.0681(6)	0.8679(4)	3.92

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Table S2. continued

C(19)	0.6314(8)	1.2009(6)	0.8604(5)	4.90
C(20)	0.6421(7)	1.2583(6)	0.9265(5)	4.04
C(21)	0.6786(7)	1.1866(6)	0.9957(5)	3.84
C(22)	0.7042(6)	1.0548(6)	1.0008(4)	3.02
C(23)	1.0505(6)	0.7926(5)	0.8805(4)	2.71
C(24)	1.1121(6)	0.9152(5)	0.8406(4)	2.59
C(25)	1.2418(6)	0.9089(6)	0.7916(4)	2.96
C(26)	1.2998(7)	1.0186(7)	0.7567(4)	3.79
C(27)	1.2286(8)	1.1355(7)	0.7705(6)	5.18
C(28)	1.0992(9)	1.1423(7)	0.8199(6)	5.92
C(29)	1.0414(7)	1.0344(7)	0.8522(6)	5.05
C(30)	1.1292(5)	0.6945(5)	0.7005(4)	2.67
C(31)	1.1440(5)	0.6135(6)	0.6308(4)	2.61
C(32)	1.1498(7)	0.6679(7)	0.5469(4)	3.90
C(33)	1.1613(8)	0.5954(9)	0.4831(5)	5.06
C(34)	1.1677(7)	0.4643(9)	0.5037(6)	5.19
C(35)	1.1638(7)	0.4072(7)	0.5876(6)	4.94
C(36)	1.1535(7)	0.4801(6)	0.6509(5)	3.96
C(37)	0.8905(6)	0.9251(5)	0.6612(4)	2.67
C(38)	0.8028(6)	0.9774(5)	0.5990(4)	2.71
C(39)	0.6943(7)	1.0739(6)	0.6166(4)	3.84
C(40)	0.6143(7)	1.1199(8)	0.5586(6)	4.85
C(41)	0.6434(8)	1.0664(8)	0.4861(6)	5.18

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Table S2. continued

C(42)	0.7499(9)	0.9730(7)	0.4658(5)	5.02
C(43)	0.8274(7)	0.9277(6)	0.5238(4)	3.69

[a] $B(eqv) = (8\pi^2/3)[a^2U_{11}(a^*)^2 + b^2U_{22}(b^*)^2 + c^2U_{33}(c^*)^2 + ab(\cos\gamma)U_{12}a^*b^* + ac(\cos\beta)U_{13}a^*c^* + bc(\cos\alpha)U_{23}b^*c^*]$

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Table S3. Final Fractional Coordinates for
(η4-C5HBz5)Fe(CO)3

Atom	x/a	y/b	z/c
H(1)[C(8)]	0.866	0.746	0.663
H(1)[C(9)]	0.565	0.797	0.851
H(2)[C(9)]	0.595	0.881	0.761
H(1)[C(11)]	0.492	0.599	0.871
H(1)[C(12)]	0.421	0.444	0.817
H(1)[C(13)]	0.434	0.467	0.673
H(1)[C(14)]	0.540	0.629	0.577
H(1)[C(15)]	0.616	0.781	0.631
H(1)[C(16)]	0.642	0.815	0.959
H(2)[C(16)]	0.773	0.817	0.985
H(1)[C(18)]	0.648	1.025	0.824
H(1)[C(19)]	0.610	1.250	0.811
H(1)[C(20)]	0.622	1.348	0.924
H(1)[C(21)]	0.685	1.228	1.040
H(1)[C(22)]	0.731	1.004	1.049
H(1)[C(23)]	1.002	0.802	0.938
H(2)[C(23)]	1.117	0.720	0.880
H(1)[C(25)]	1.292	0.828	0.780
H(1)[C(26)]	1.391	1.011	0.725
H(1)[C(27)]	1.268	1.209	0.743
H(1)[C(28)]	1.051	1.224	0.832
H(1)[C(29)]	0.950	1.040	0.885

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Table S3. continued

H(1)[C(30)]	1.183	0.650	0.738
H(2)[C(30)]	1.162	0.772	0.673
H(1)[C(32)]	1.146	0.758	0.533
H(1)[C(33)]	1.164	0.635	0.426
H(1)[C(34)]	1.177	0.411	0.461
H(1)[C(35)]	1.167	0.317	0.601
H(1)[C(36)]	1.151	0.440	0.708
H(1)[C(37)]	0.982	0.926	0.630
H(2)[C(37)]	0.868	0.980	0.704
H(1)[C(39)]	0.676	1.110	0.668
H(1)[C(40)]	0.539	1.184	0.570
H(1)[C(41)]	0.590	1.096	0.446
H(1)[C(42)]	0.770	0.937	0.414
H(1)[C(43)]	0.902	0.862	0.511

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Table S4. Thermal Parameters for

(η4-C5HBz5)Fe(CO)3

Atom	U11	U22	U33	U12	U13	U23
Fe	0.0426(5)	0.0277(4)	0.0287(4)	-0.0063(3)	-0.0100(3)	-0.0015(3)
O(1)	0.072(3)	0.069(3)	0.061(3)	-0.015(3)	-0.018(3)	-0.033(3)
O(2)	0.088(4)	0.071(3)	0.048(3)	-0.040(3)	0.011(3)	0.006(2)
O(3)	0.082(4)	0.063(3)	0.085(4)	0.017(3)	-0.047(3)	-0.014(3)
C(1)	0.045(4)	0.041(3)	0.047(4)	-0.009(3)	-0.012(3)	-0.004(3)
C(2)	0.058(4)	0.029(3)	0.056(4)	-0.012(3)	-0.022(3)	-0.004(3)
C(3)	0.066(4)	0.034(3)	0.042(4)	-0.014(3)	-0.017(3)	0.007(3)
C(4)	0.034(3)	0.029(3)	0.033(3)	-0.003(2)	-0.011(2)	-0.004(2)
C(5)	0.040(3)	0.028(3)	0.028(3)	-0.009(2)	-0.005(2)	0.002(2)
C(6)	0.047(3)	0.024(3)	0.041(3)	-0.009(2)	-0.019(3)	0.001(2)
C(7)	0.039(3)	0.029(3)	0.026(3)	-0.009(2)	-0.006(2)	0.000(2)
C(8)	0.042(3)	0.035(3)	0.022(3)	-0.007(2)	-0.007(2)	-0.001(2)
C(9)	0.040(3)	0.037(3)	0.044(4)	0.000(3)	-0.008(3)	-0.007(3)
C(10)	0.031(3)	0.038(3)	0.046(4)	-0.002(2)	-0.012(3)	-0.003(3)
C(11)	0.043(4)	0.043(3)	0.042(4)	-0.002(3)	-0.009(3)	0.000(3)
C(12)	0.063(5)	0.047(4)	0.066(5)	-0.015(3)	-0.018(4)	0.003(3)
C(13)	0.052(4)	0.060(5)	0.099(7)	-0.006(4)	-0.031(4)	-0.029(4)
C(14)	0.062(5)	0.095(6)	0.042(4)	-0.010(4)	-0.019(4)	-0.014(4)
C(15)	0.046(4)	0.063(4)	0.033(3)	-0.013(3)	-0.008(3)	0.001(3)
C(16)	0.050(4)	0.039(3)	0.034(3)	-0.003(3)	-0.005(3)	-0.011(3)
C(17)	0.041(3)	0.039(3)	0.042(3)	-0.005(3)	-0.009(3)	-0.008(3)
C(18)	0.108(6)	0.037(4)	0.047(4)	0.000(4)	-0.033(4)	-0.013(3)

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Table S4. continued

C(19)	0.125(7)	0.040(4)	0.074(6)	0.002(4)	-0.044(5)	-0.008(4)
C(20)	0.076(5)	0.037(4)	0.080(6)	0.000(3)	-0.010(4)	-0.026(4)
C(21)	0.071(5)	0.048(4)	0.071(5)	0.002(3)	-0.026(4)	-0.030(4)
C(22)	0.055(4)	0.050(4)	0.042(4)	-0.003(3)	-0.011(3)	-0.016(3)
C(23)	0.057(4)	0.045(3)	0.031(3)	-0.012(3)	-0.017(3)	-0.003(3)
C(24)	0.043(4)	0.044(3)	0.041(3)	-0.007(3)	-0.018(3)	-0.008(3)
C(25)	0.050(4)	0.054(4)	0.040(4)	-0.003(3)	-0.016(3)	-0.011(3)
C(26)	0.050(4)	0.069(5)	0.064(5)	-0.016(4)	-0.018(4)	0.006(4)
C(27)	0.071(6)	0.051(5)	0.131(8)	-0.018(4)	-0.038(5)	0.003(5)
C(28)	0.080(6)	0.041(4)	0.16(1)	-0.008(4)	-0.022(6)	-0.015(5)
C(29)	0.047(4)	0.052(4)	0.143(8)	-0.009(4)	-0.005(5)	-0.033(5)
C(30)	0.040(3)	0.049(3)	0.042(3)	-0.009(3)	-0.014(3)	-0.009(3)
C(31)	0.028(3)	0.056(4)	0.043(4)	-0.007(3)	-0.002(3)	-0.018(3)
C(32)	0.064(5)	0.074(5)	0.051(4)	-0.015(4)	-0.012(4)	-0.009(4)
C(33)	0.086(6)	0.116(7)	0.046(5)	-0.022(5)	-0.012(4)	-0.025(5)
C(34)	0.071(5)	0.109(7)	0.074(6)	-0.020(5)	0.008(4)	-0.061(6)
C(35)	0.078(6)	0.065(5)	0.097(7)	-0.013(4)	-0.003(5)	-0.042(5)
C(36)	0.062(5)	0.060(4)	0.070(5)	0.000(4)	-0.015(4)	-0.022(4)
C(37)	0.053(4)	0.039(3)	0.039(3)	-0.016(3)	-0.018(3)	0.003(3)
C(38)	0.051(4)	0.041(3)	0.038(3)	-0.019(3)	-0.014(3)	0.018(3)
C(39)	0.069(5)	0.057(4)	0.054(4)	-0.012(4)	-0.015(4)	0.021(3)
C(40)	0.056(5)	0.082(6)	0.089(6)	-0.002(4)	-0.021(5)	0.026(5)
C(41)	0.080(6)	0.092(6)	0.084(6)	-0.039(5)	-0.051(5)	0.041(5)

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Table S4 continued

C(42)	0.117(7)	0.073(5)	0.061(5)	-0.044(5)	-0.054(5)	0.023(4)
C(43)	0.076(5)	0.059(4)	0.047(4)	-0.026(4)	-0.027(4)	0.013(3)

Anisotropic thermal parameters are defined by exp[-2pi(pi)(hha*a*U11 + kkb*b*U22 + 11c*c*U33 + 2hka*b*U12 + 2klb*c*U23 + 2hla*c*U13)].

Hydrogen atoms were given a fixed isotropic thermal parameter of B = 5.5 angstroms squared.

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Table S5. Least-Squares Planes for
(η4-C5HBz5)Fe(CO)3

Equation of Plane 1: (0.1126)X + (0.8899)Y + (-0.4420)Z = (4.8836)

Atom	Deviation	
C4	0.00597	[The first 4 atoms define plane 1.]
C5	-0.00945	
C6	0.00949	
C7	-0.00599	
FE	-1.72243	
C8	0.58451	
C9	0.03485	
C16	-0.01171	
C23	0.10694	
C30	0.04785	

Equation of Plane 2: (0.7886)X + (-0.6043)Y + (-0.1139)Z = (1.8117)

Atom	Deviation	
C10	0.00815	[The first 6 atoms define plane 2.]
C11	-0.00502	
C12	-0.00477	
C13	0.01142	
C14	-0.00811	
C15	-0.00166	
C9	-0.02976	

Equation of Plane 3: (0.8850)X + (-0.0117)Y + (-0.4654)Z = (5.2253)

Atom	Deviation	
C17	0.00954	[The first 6 atoms define plane 3.]
C18	-0.01203	
C19	0.00796	
C20	-0.00165	
C21	-0.00060	
C22	-0.00322	
C16	0.01946	

Equation of Plane 4: (-0.5616)X + (-0.0582)Y + (-0.8254)Z = (-21.2517)

Atom	Deviation	
C24	-0.00934	[The first 6 atoms define plane 4.]
C25	-0.00130	
C26	0.00421	
C27	0.00343	
C28	-0.01442	
C29	0.01738	

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C23 -0.04845

Equation of Plane 5: (0.9702)X + (-0.1217)Y + (-0.2093)Z = (12.7581)

Atom	Deviation	
C31	-0.01064	[The first 6 atoms define plane 5.]
C32	0.00451	
C33	0.00358	
C34	-0.00537	
C35	-0.00099	
C36	0.00891	
C30	-0.03211	

Equation of Plane 6: (0.6249)X + (0.6266)Y + (-0.4657)Z = (11.2163)

Atom	Deviation	
C38	0.00162	[The first 6 atoms define plane 6.]
C39	-0.00096	
C40	0.00578	
C41	-0.01116	
C42	0.01146	
C43	-0.00675	
C37	-0.01711	

Equation of Plane 7: (0.1664)X + (0.9393)Y + (-0.2999)Z = (5.3177)

Atom	Deviation	
C1	0.00000	[The first 3 atoms define plane 7.]
C2	0.00000	
C3	0.00000	
FE	0.88967	

The angle between plane 1 and plane 2 is 113.49.
The angle between plane 1 and plane 3 is 72.85.
The angle between plane 1 and plane 4 is 75.54.
The angle between plane 1 and plane 5 is 84.64.
The angle between plane 1 and plane 6 is 33.50.
The angle between plane 1 and plane 7 is 9.16.
The angle between plane 2 and plane 3 is 40.71.
The angle between plane 2 and plane 4 is 108.28.
The angle between plane 2 and plane 5 is 30.40.
The angle between plane 2 and plane 6 is 80.38.
The angle between plane 2 and plane 7 is 113.72.
The angle between plane 3 and plane 4 is 96.44.
The angle between plane 3 and plane 5 is 16.76.
The angle between plane 3 and plane 6 is 40.32.
The angle between plane 3 and plane 7 is 73.99.
The angle between plane 4 and plane 5 is 111.41.
The angle between plane 4 and plane 6 is 90.17.
The angle between plane 4 and plane 7 is 84.30.

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The angle between plane 5 and plane 6 is  51.13.
The angle between plane 5 and plane 7 is  83.68.
The angle between plane 6 and plane 7 is  33.67.
      1.734       3.016       1.807
The Centl FE    C1    angle is 116.81.
      1.734       3.068       1.792
The Centl FE    C2    angle is 120.95.
      1.734       3.068       1.777
The Centl FE    C3    angle is 121.81.
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